

## Numbering scheme for compound codes (NRDC2023 A8)

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### Note added to WP2024-11:

The compound flag \* is given to all compound codes defined in Dictionary 209. Is there any program using this flag? If not, I would like to eliminate this flag from the dictionary thoroughly.

I reviewed the current numbering scheme of the compound codes defined in Dictionary 209. This number is an integer (16), of which the first three digits are for the atomic number (similar to numbering of a nuclide in Dictionary 227) and the last three digits are defined as summarized below:

Current	Change to?	Symbol	Explanation
130	430	ALY	alloy
137	437	HYD	hydride
300	500	AIR	air
310	510	AMM	ammonium
320	520	BNZ	benzene
330	530	CMP	compound (general)
340	540	CXX	organic compound (general)
350	550	D2O	heavy water
360	560	DXX	deuterium compound
370	570	ARM	aromatic compound
380	580	MTH	methyl compound
390	590	OXI	oxide
400	600	PFN	paraffin
410	610	PHL	phenyl compound
420	620	PLE	polyethylene
430	630	TXX	tritium compound
440	640	WTR	water
450	650	BUT	butyl compound
460	660	ETH	ethyl compound
470	670	PRO	propyl compound

I would like to suggest the following changes:

- increase the first digit characterizing the compound to avoid interference with the mass number (up to ~300)
- add “0” as the seventh digit (to be consistent with Dictionary 227 for nuclide codes)

### Examples

Code	Current	Change to?	Explanation
40-ZR-ALY	40130	404300	Zircalloy
40-ZR-CMP	40330	405300	Zirconium compound (general)
40-ZR-HYD	40137	404370	Zirconium hydride
40-ZR-OXI	40390	405900	Zirconium oxide
40-ZR-0	400000		Natural zirconium
40-ZR-90-G	400900		Zirconium-90 (ground state)
40-ZR-90-M	400901		Zirconium-90 (metastable state)
40-ZR-91	400910		Zirconium-91

**Dictionary 209: Compounds (Proposed change)**

<b>Line</b>	<b>Contents</b>	<b>Format</b>	<b>Archive</b>	<b>Trans</b>	<b>CHEX</b>
1	Code	A10	13-22	1-10	x
	CINDA code	A5	44-48	N/A	
	Internal numerical equivalent	I7	49-55	N/A	x
	<del>(Field not currently used)</del>	<del>A13</del>	<del>55-67</del>	<del>N/A</del>	
	<del>(presently not in use)</del>	<del>E5</del>	<del>68-72</del>	<del>N/A</del>	
	<del>(presently not in use)</del>	<del>E11</del>	<del>73-83</del>	<del>N/A</del>	
	Expansion	A25	84-108	(12-38)	
	Compound flag * compound	A1	114	N/A	
2+	<del>Output dictionary number for DANIEL</del> <del>(presently not used)</del>	<del>I2</del>	<del>44-45</del>	<del>N/A</del>	
	Comment	A55	46-100	12-66	